Chemistry: Review: Formulas

Atomic Mass

Relative mass of an average atom of an element. Example: carbon – 12 atoms used as reference.[C-12 atom: mass of atomic mass unit.]

Molecular Mass

Is the sum of the atomic masses of the atoms in a molecules. Molecular mass is measured in the unit μ or g mol^{-1}

Formula Mass

Ionic compounds do not exist in the force of molecules
Sum of the atomic masses of the ions present in the simplest formula or formulas unit of an ionic compound.

Avogadro's number

1 mole is 6.022045×10^{23} particles of the substance
The mole is the SI unit for amount of substance, and its symbol is: mol.

$$\boxed{NumberOfParticles = \#\,mol \times 6.02 \times 10^{23}}$$

1 mole = One molecular mass in grams = One formula mass in gram

$$NumberOfMol = \frac{MassGrams(g)}{MolarMass(\mu)}$$

Percentage composition

Tells the chemist how much of each element or each polyatomic ion is present in a compound on a percent base.

$$\boxed{PercentOfElement = \frac{AtomicMassOfNumberOfAtomsInFormula}{MolarMassOfCompound} \times 100}$$

Example: What is the percentage of each element in $CH_3CH_2NH_2$?

Empirical Formulas

Is the simplest ratio of atoms in a chemical compound
Molecular formula is always a whole number multiple of the empirical formula
[e.g. CH for C_2H_2, or C_6H_6]

Determining empirical formulas:

1. Assume 100% = 100 grams
2. Calculate the moles of each element in the compound from the given data.
3. Divide the number of moles of each element found in step 2 by the smallest of these values, to obtain whole number subscripts for the empirical formula
4. If step 3 does not give whole numbers the answers should be multiplied by some number to obtain whole number ratios

Examples of calculation of empirical formula

An organic compound contains 92.25% carbon and 7.75% hydrogen. What is the empirical formula?

NOTE: in writing empirical formulas, the least electronegative element is written first (the first element should be the one closest to the left edge of the Periodic Table). For organic compounds: Carbon is always first, hydrogen second and oxygen third, then any other elements.

Molecular formulas

An empirical formula gives the simplest ratio of atoms in a molecule.
The molecular formula indicates not only the ratio of the atoms of the elements in a compound but also the actual number of atoms of each element in one molecule of the compound.

The number of empirical formula units in a molecular formula is determined by:

$$\boxed{\frac{MolarMass}{MolarMassO\quad fEmpirical\quad Formula} = SmallWhole\quad Number}$$

Each subscript in the empirical formula is then multiplied by this small whole number to obtain the molecular formula.

Stoichiometry Calculations

Study of the quantitative relationships in chemical reaction.
These calculations allow the chemist to predict the result of a chemical reaction in terms of the mass or moles of products produced and reactants consumed

Steps of calculations

1. **Balanced equation**
2. **Grams to mole**
3. **Mole to mole ratio**
4. **Reverse step 2; mole to gram conversion**

Example:
If 100.0g propane, C_3H_8 undergo combustion in excess oxygen, what mass will be needed, how many grams of carbon dioxide and water will be formed in the reaction?

Start with grams given → grams to mols → use mol ratio → mols to grams → end with grams required

Answer: 364g O_2, 300g CO_2, 164g H_2O

Percentage Yield

$$\%Yield = \frac{Experiment\,al Yield}{Theoretica\,l Yield} \times 100$$

Theoretical Yield

Theoretical Yield is the maximum amount of product formed in the reaction, determined by calculation from a balanced equation using mol : mol ratio.

Percentage Error

$$\%Error = \frac{\left| TheoreticalYield - ExperimentalYield \right|}{TheoreticalYield} \times 100$$

Limiting Reagent

When the amounts of two or more reactants are given in the statement of the problem. Then use procedures for solving limiting reactant problems
Identify the limiting reagent from calculations then follow the same procedure as for stoichiometric calculation, except remember to use the moles of the limiting reagent for mole to mole ratio.

Calculations in Solution chemistry : conc. = no. moles ÷ vol (dm^3)

Molarity (M) is a unit of concentration meaning one mole per liter, or in $moldm^{-3}$.

A standard solution

A standard solution is a solution in which a precise mass of solute is being dissolved in a precise volume of a solvent, therefore the concentration is precisely known.

The total number of particles changes when the volume is changed but the concentration of the particle (the number of the particles per unit volume.) does not change

Dilution is the process whereby pure solvents is added to a solution in order to decrease the concentration of the solute

Concentrated = Dilute
Stock (before) = Stock (after)
$C_1V_1 = C_2V_2$
$C_{before}\,V_{before} = C_{after}\,V_{after}$

Solution Stoichiometry Calculations

Same step as above for the mass calculations

Titration Problems:

Titration is neutralization between an acid and a base with the use of an indicator. The calculations are the same as the solution Stoichiometry.

Burette
Pipette
End Point
Equivalence Point
Volumetric Analysis
Gravimetric analysis

Calculations of Acid and Base concentrations

$$2\ H_2O \rightleftharpoons H_3O^+ + OH^-$$

$$K_w = [H_3O^+][OH^-] = 1 \times 10^{-14} \text{ at } 25\ ^0C$$

$$pH = -\log [H^+] \qquad [H^+] = 10^{-pH}$$

$$pOH = -\log [OH^-] \qquad [OH^-] = 10^{-pOH}$$

$$pH + pOH = 14$$

Writing Net - Ionic Equations

1. Write a balanced molecular equation, including the states.
2. Write the complete dissociated ionic equation representing the precipitate and all ions in aqueous solution. (Recall: solids, liquids, and gases do not dissociate)
3. Eliminate the spectator ions (i.e. those ions that do not take part in the reaction) from both sides of the equation.
4. Write the overall net ionic equation (containing no spectator ions).

To work out which is the precipitate in a double displacement reacion, use the solubility chart, (Recall: Generally all nitrates, all Group I compounds, all ammonium compounds, all chlorate, all perchlorate, and all acetates are soluble)

Example: Write the net ionic equation for the following reaction:

$$FeCl_{3(aq)} + 3\ NaOH_{(aq)} \Rightarrow Fe(OH)_{3\ (s)} + 3\ NaCl_{(aq)}$$

Bronsted - Lowry Definition of acids and bases:

Conjugate acid and Conjugate Base:

Strong acid/base vs. weak

Testing for strong and weak electrolytes

concentrated vs. dilute

GASES

1.**BOYLE'S LAW** 2.**CHARLES' LAW GAY/LUSSAC** 3.**GAY-LUSSAC LAW**

P α 1/v [inverse or indirect] V α T (K) [n, P constant] P α T [n, v constant]

[n T constant]

273ºC = O K

Every ºC = 1K

$P_1V_1 = P_2V_2$

T(K) = t (ºC) = 273

$\frac{P_1}{T_1} = \frac{P_2}{T_2}$

(2 x P = ½ v or ½ v =2P)

[note: V=0 at absolute zero]

A graph of P against 1/V is a straight line passing through the origin.

$\frac{V_1}{T_1} = \frac{V_2}{T_2}$

(T = Kelvin, 2 x T = 2 x V)

(2T = 2P)

DALTON'S LAW OF PARTIAL PRESSURE

The total pressure of a mixture of gases equals the sum of the partial pressure of each gas in the mixture.

$$\frac{\text{Moles of gas 1}}{\text{Total molesof gas}} = \frac{\text{partial pressure of gas, } p_1}{\text{Total pressure, } P_T} \quad \text{therefore} = \frac{\text{\#moles gas 1 x } P_T}{\text{Total moles}}$$

partial pressure of gas1, p_1 = mole fraction of gas 1 x P_T

$$p_1 = \frac{n_1}{n_2} \times P_T$$

Also we can use the ideal gas equation: $\mathbf{P_TV = n_T RT}$

P_T = sum of partial pressures of the gaseous mixture.

n_T = total # of moles of all gases present in the mixture.

Graham's Law: The rates of diffusion of two gases are inversely proportional to the square root of their Molar Mass. i.e.

$$\frac{\text{Rate of diffusionof A}}{\text{Rate of diffusion of B}} = \text{the square root of } \frac{\text{Molar mass of B}}{\text{Molar mass of A}}$$

$$\frac{RateofdiffusionofA}{RateofdiffusionofB} = \sqrt{\frac{molarmassofB}{molarmassofA}}$$

Combined or General Gas Equation

$$\frac{P_1V_1}{T1} = \frac{P_2V_2}{T2}$$ (T = Kelvin)

Used generally when a gas is described under **2 sets of different conditions.**

IDEAL GAS EQUATION: This equation applies only for ideal gases.

The equation is: **$PV = n\,RT$**

Any gas that obeys this equation is called an Ideal Gas.
PV = n RT is applied to a single set of conditions
R = 0.082 L. atm/mol. K, = 8.31 L. kPa / mol K
R = Avogadro's constant = Ideal (Universal) Gas Constant, is the same for all gases.
The value for 'R' is always given on the examination paper.

$n = \frac{m}{MM}$ therefore, $PV = \frac{m}{MM} \times RT$

For a mixture of gases: $P_T V = n_T R_T$

$\text{density} = \frac{\text{mass}}{\text{volume}}$ therefore, $P = \frac{d \times RT}{MM}$

Therefore density and/or the molar Mass of an unknown gas may be easily calculated.

Gas volumes are usually compared at **0 ^{O}C and 101.3 kPa**. These conditions are referred to as **standard temperature and pressure, stp**. Avogadro in 1811 suggested:
"equal volumes of gases measured at the same conditions of temperature and pressure contain the same number of molecules ".

It follows from Avogadro's hypothesis that if equal volumes of gases contain equal numbers of molecules then the volume occupied by one mole of molecules must be the same for all gases.

It is called the **gas molar volume**. The value is **22.414 dm^3 at stp** (0 ^{O}C and 101.3 kPa).

$$\text{number of molesof gas} = \frac{\text{Volume in litres}}{\text{Volume at STP (22.4L)}}$$

Thermochemistry

Elements in their standard state, (i.e at 25 ^{O}C and 101.3 kPa), are regarded as having zero enthalpy, i.e. they are by convention assumed to have a heat content of zero.

$$\text{Heat Capacity, C} = \frac{\text{Heat Absorbed, or released by an object, Q}}{\text{Increase in Temperature, } \Delta T}$$

$$\text{Specific Heat, c} = \frac{\text{Heat Capacity, C}}{\text{Mass, m}}$$

Heat Energy, Q = (Mass, m) x (Specific Heat, c) x (Change in Temperature, ΔT)

$$\mathbf{Q = m\,c\,\Delta T}$$

Molar Heat capacity = specific heat capacity x molar mass (J/mol ^{O}C)

Hess' Law: Energy conservation is the basis of **Hess's Law**, which states that, if a reaction is the sum of two or more other reactions, then ΔH for the overall process must be the sum of the ΔH values of the constituent reactions.

The enthalpy change for a chemical or physical change does not depend on the path you choose to go from the initial conditions to the final conditions.

The equation below can be used to find the standard enthalpy change for a reaction, ΔH°_{rxn}:

Enthalpy change for a reaction = $\Delta H^\circ_{rxn} = \Sigma\ [\Delta H^\circ_f \text{ (products)}] - \Sigma\ [\Delta H^\circ_f \text{ (reactants)}]$

Standard enthalpy change = standard enthalpy of products - Standard enthalpy of reactants

The standard enthalpy of a substance = its standard enthalpy of formation

The **bond dissociation energy, D,** is the enthalpy change for breaking a bond in a molecule with the reactants and products in the gas phase under standard conditions.
For the diatomic molecule XY, the bond dissociation energy is defined as the enthalpy change for the process: $XY_{(g)} \longrightarrow X_{(g)} + Y_{(g)}$

When using bond energies to find the enthalpy change for a reaction, you should add up the energies of all the bonds broken and subtract from this the sum of the energies of the bonds formed. Thus, the **standard enthalpy of reaction is the difference between the sum of the average standard bond enthalpies of the products and the sum of the average standard bond enthalpies of the reactants**:

$$\Delta H^0_{rxn} = \Sigma\ D \text{ (bonds broken)} - \Sigma\ D \text{ (bonds formed)}$$

This equation tells you to multiply the bond energy for each bond broken by the number of bonds of that type, and add all of these up. Then, multiply the bond energy for each bond formed by the number of bonds of that type, and add all of these up.

Constructing a Born-Haber Cycle: Formation of $MX_{(s)}$ from $M_{(s)}$ and ½ $X_{2(g)}$

$$M_{(s)} \xrightarrow{(1)\ =\ \Delta H^0_S} M_{(g)}$$

$$M_{(g)} + e^{-1} \xrightarrow{(2)\ =\ I.E_1} M^{+1}_{(g)}$$

$$\tfrac{1}{2} X_{2\,(g)} \xrightarrow{(3)\ =\ \frac{1}{2}\Delta H^0 (D)} X_{(g)}$$

$$X_{(g)} \xrightarrow{(4)\ =\ E.\ A_1} X^{-1}_{(g)} + e^{-1}$$

$$M_{(s)} + \tfrac{1}{2} X_{2(g)} \xrightarrow{(5)\ =\ \Delta H_f^0} MX_{(s)}$$

$$M^{+1}_{(g)} + X^{-1}_{(g)} \xrightarrow{(6)\ =\ \Delta H^0_L} MX_{(s)}$$

(1) = ΔH^0_S = energy of atomisation, ΔH^0_S, measured by direct calorimetry
(2) = $I.E_1$ = ionisation energy, $I.E_1$, measured from spectroscopy
(3) = ½ ΔH^0 (D) = ½ bond dissociation energy, ½ ΔH^0 (D), measured directly from enthalpy of rxn.
(4) = E. A_1 = electron affinity, $E.A_1$, difficult to measure directly
(5) = ΔH_f^0 = enthalpy of formation of 1 mole of compound from its constituent elements
(6) = ΔH^0_L = standard Lattice Enthalpy, difficult to measure directly, the energy required to decompose 1 mole of an ionic compound

Standard Enthalpy of Formation, ΔH_f^0 (MX) = $\Delta H_s^0 + I.E_1 + \frac{1}{2} D + E.A_1 + \Delta H_L$